

Dimethyl sulfoxide
67-68-5 | DTXSID2021735

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.98e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.51e-01

Confidence level: 4.96e-01

Nearest Neighbors from the Training Set

Image not found

Chloroform

Measured: 6.10e-01

Predicted: 319

Image not found

Butanoic acid, 3-methyl-, methyl ester

Measured: 12.1

Predicted: 14.5

Image not found

Propaphos

Measured: 1.45

Predicted: 2.83e-06

Image not found

1-Chlorohexane

Measured: 8.24e-03

Predicted: 19.3